Appln No.: 09/373,018
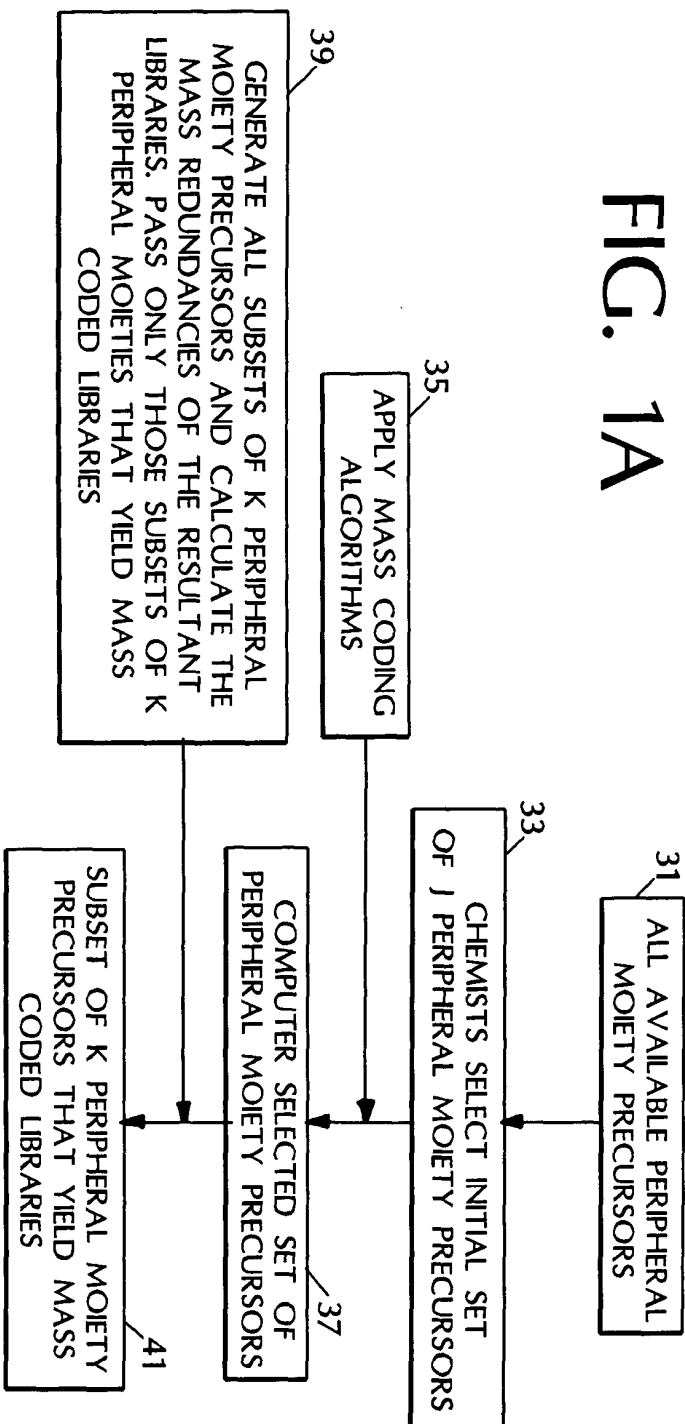Applicant(s): Huw M. Nash, et al.
METHOD FOR PRODUCING AND SCREENING MASS-
CODED COMBINATORIAL LIBRARIES FOR DRUG
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MASS CODING FLOWCHART

FIG. 1A

31 — ALL AVAILABLE PERIPHERAL MOIETY PRECURSORS

33 — CHEMISTS SELECT INITIAL SET OF J PERIPHERAL MOIETY PRECURSORS

35 — APPLY MASS CODING ALGORITHMS

37 — COMPUTER SELECTED SET OF PERIPHERAL MOIETY PRECURSORS

39 — GENERATE ALL SUBSETS OF K PERIPHERAL MOIETY PRECURSORS AND CALCULATE THE MASS REDUNDANCIES OF THE RESULTANT LIBRARIES. PASS ONLY THOSE SUBSETS OF K PERIPHERAL MOIETIES THAT YIELD MASS CODED LIBRARIES

41 — SUBSET OF K PERIPHERAL MOIETY PRECURSORS THAT YIELD MASS CODED LIBRARIES

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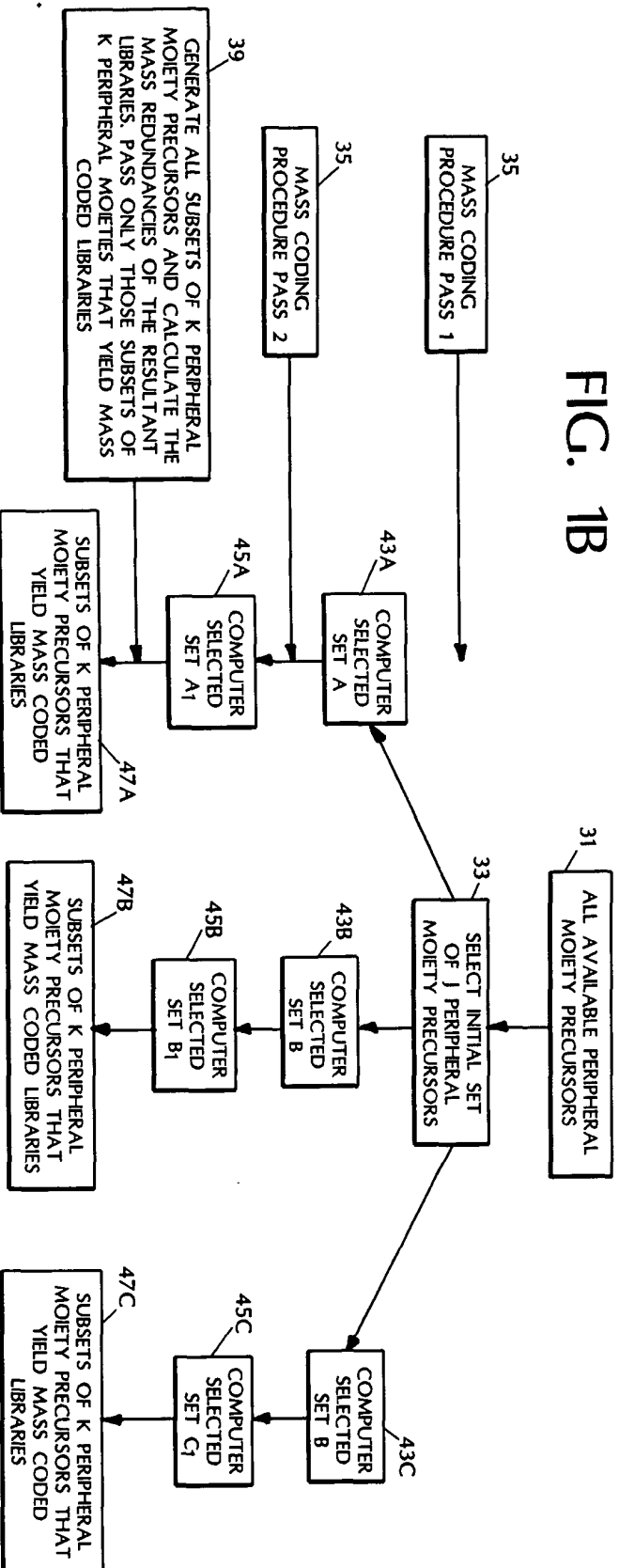METHOD FOR PRODUCING AND SCREENING MASS-CODED COMBINATORIAL LIBRARIES FOR DRUG DISCOVERY AND TARGET VALIDATION

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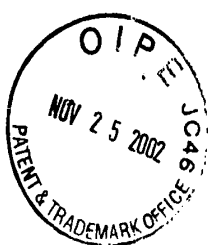ALTERNATE METHOD FOR MASS CODING

FIG. 1B

% MASS REDUNDANCY OF LIBRARIES FROM A COMPUTER SELECTED SET OF PERIPHERAL MOIETY PRECURSORS

Library Mass Redundancy	Number of Libraries	Percentage of Set
<3%	24	1.32
<5%	234	12.86
<10%	972	53.41

Average Mass Redundancy	11.47 Percent

NUMBER OF LIBRARIES WITH ≤ % MASS REDUNDANCY

FIG. 2A

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CODED COMBINATORIAL LIBRARIES FOR DRUG
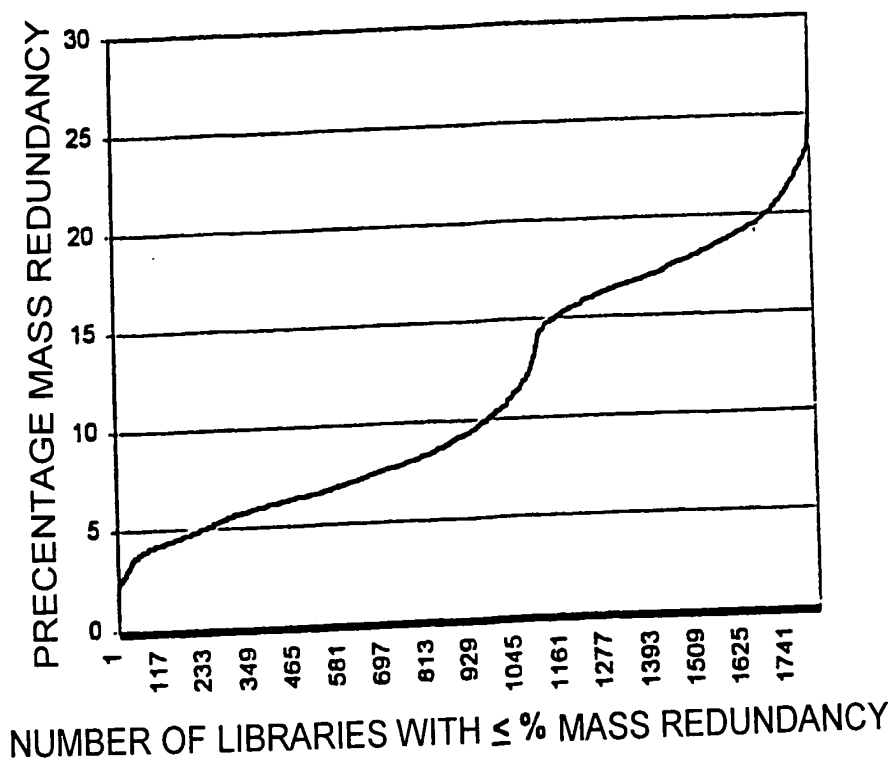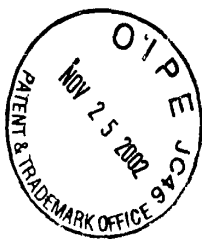DISCOVERY AND TARGET VALIDATION

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% MASS REDUNDANCY OF LIBRARIES FROM A RANDOMLY CHOSEN SET OF PERIPHERAL MOIETY PRECURSORS

Library Mass Redundancy	Number of Libraries	Percentage of Set
<3%	0	0.00
<5%	0	0.00
<10%	0	0.00

Average Mass Redundancy	60.69 Percent

FIG. 2B

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PRECENTAGE MASS REDUNDANCY

Percentage Mass Redundancy of Libraries

NUMBER OF LIBRARIES WITH ≤ % MASS REDUNDANCY

From Randomly Chosen Set

COMPARISON OF THE PERCENTAGE MASS
REDUNDANCY OF LIBRARIES OBTAINED FROM
A COMPUTER SELECTED SET OF PERIPHERAL
MOIETY PRECURSORS vs THOSE OBTAINED
FROM A RANDOMLY CHOSEN SET OF
PERIPHERAL MOIETY PRECURSORS
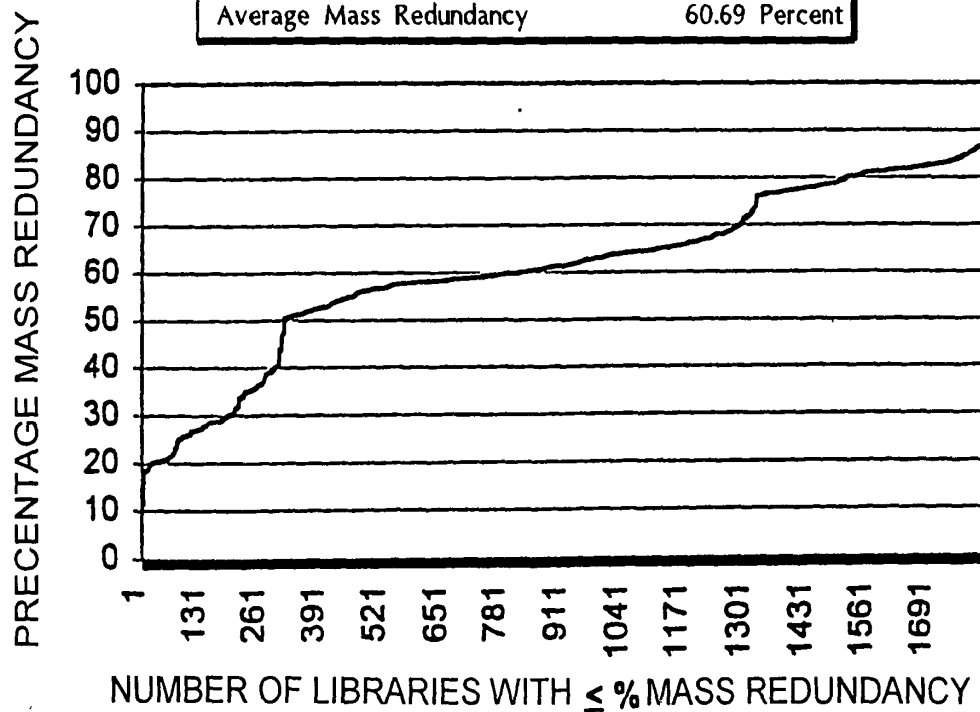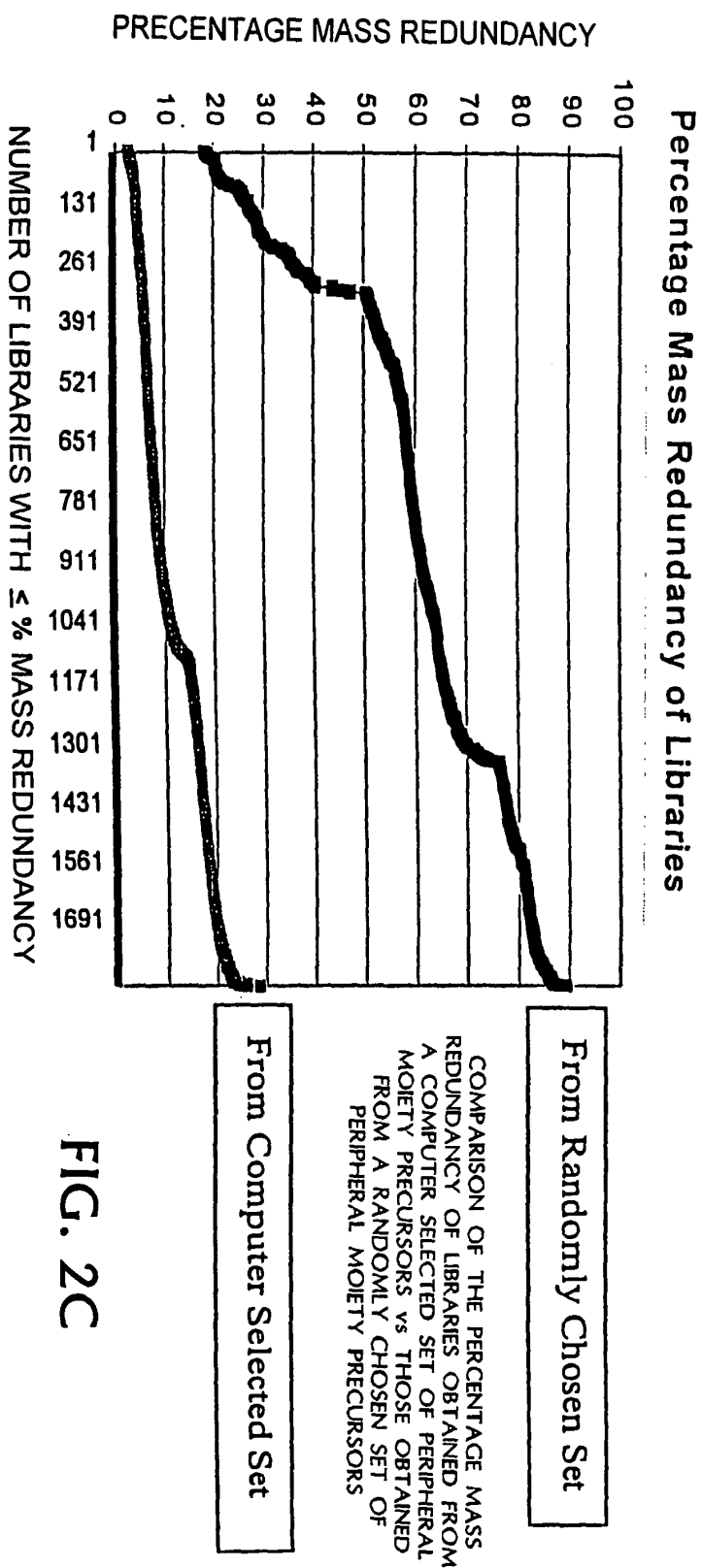
From Computer Selected Set

FIG. 2C

Appln No.: 09/373,018
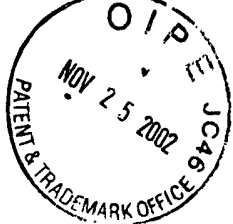Applicant(s): Huw M. Nash, et al.
METHOD FOR PRODUCING AND SCREENING MASS-
CODED COMBINATORIAL LIBRARIES FOR DRUG
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PERIPHERAL MOIETY
PRECURSORS STORED IN DATABASE
OR ELECTRONIC DATA STORAGE SYSTEM

13

COMPUTER SELECTS
FOR USER SET
CRITERIA, DIVERSITY,
SIZE, SHAPE, ETC.

19

HUMAN SELECTION
(VIA 21)

15

INPUT₁

INITIAL SET OF PERIPHERAL
MOIETY PRECURSORS STORED
IN COMPUTER OR ELECTRONIC
DATA STORAGE SYSTEM

29

11

OUTPUT₁

INPUT₂

27

MASS CODING PROCESS

COMPUTER, DIGITAL OR
ANALOG PROCESS

17

OUTPUT₂

MASS CODED SETS OF PERIPHERAL
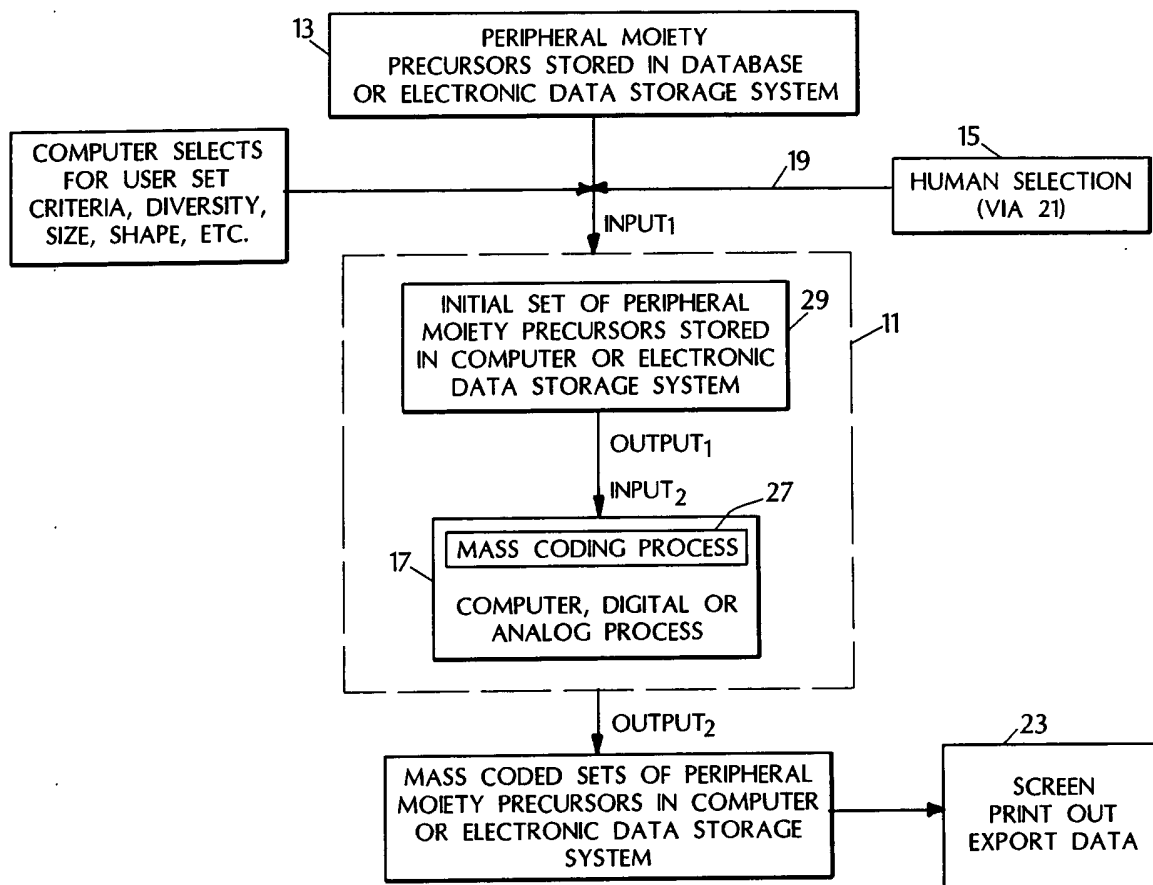MOIETY PRECURSORS IN COMPUTER
OR ELECTRONIC DATA STORAGE
SYSTEM

SCREEN
PRINT OUT
EXPORT DATA

23

SYSTEM FLOW FOR
MASS CODING PROCESS

FIG. 3